Electronic Supplementary Material (ESI) for New Journal of Chemistry
This journal is © The Royal Society of Chemistry and The Centre National de la Recherche Scientifique 2013

Supplementary Material (ESI) for New Journal of Chemistry
This journal is (c) The Royal Society of Chemistry and The Centre National de la Recherche Scientifique, 2012.

Synthesis and crystal structure of a series of Schiff bases. A photo-, solvato- and acidochromic compound†

Arturo Jiménez-Sánchez,[a] Mario Rodríguez,[b]* Rémi Métivier,[d] Gabriel Ramos-Ortíz, [b] Jose Luis Maldonado, Netzahualcoyotl de los Santos Réboles,[b] Norberto Farfán,[c] Keitaro Nakatani,[d] Rosa Santillan.[a]*

[a] *Departamento de Química, Centro de Investigación y de Estudios Avanzados del IPN, CINVESTAV, Apdo. Postal 14-740, México, D. F., 07000, México. E-mail: rsantill@cinvestav.mx; Fax: +52 555-747-3389; Tel: +52 555-747-3725*

[b] *Centro de Investigaciones en Óptica, CIO, Apdo., Postal 1-948, 37000 León Gto., México*

[c] *Facultad de Química, Departamento de Química Orgánica, Universidad Nacional Autónoma de México, México, D.F., 04510, México*

[d] *Laboratoire de Photophysique et Photochimie Supramoléculaires (UMR 8531 du CNRS), Ecole Normale Supérieure de Cachan, Avenue du Président Wilson, 94235, Cachan, France.*

To whom the correspondence should be addressed: rsantill@cinvestav.mx

Electronic Supplementary Material (ESI) for New Journal of Chemistry
This journal is © The Royal Society of Chemistry and The Centre National de la Recherche Scientifique 2013

Supplementary Information

Contents: **Page**

I Synthesis and characterization

*2.2.1. Synthesis of Schiff bases **1b-1d** and **2a-2c.***

2-[3-(4-Dimethylaminophenyl)allylideneamino]benzylalcohol (**1b**). The title compound was prepared from 4-dimethylamino-*trans*-cinnamaldehyde (1.00 g, 5.7 mmol) and 2-aminobenzyl alcohol (0.70 g, 5.7 mmol) under reflux of toluene:ethanol (15 mL:15 mL) for 3 h, to give 1.54 g (5.5 mmol, 96% yield) of **1b**. m.p.: 120-123ºC. IR (KBr) $\bar{\nu}_{max}$(cm^{-1}): 3154, 2973, 2925, 1596 (CN), 1446, 1358, 1265, 1157, 992, 947. ^{1}H NMR ($CDCl_3$, 500 MHz) δ: 8.21 (1H, d, *J* = 9.0 Hz, H-7), 7.44 (2H, d, *J* = 8.7 Hz, H-3), 7.33-7.27 (2H, m, H-10, H-2), 7.19 (1H, d, *J* = 7.3 Hz, H-11), 7.11-7.06 (2H, m, H-13, H-5), 6.93 (1H, dd, *J* = 15.7, 9.0 Hz, H-6), 6.68 (2H, d, *J* = 8.9 Hz, H-12), 4.72 (2H, s, CH_2), 3.01 (6H, s, $N(CH_3)_2$) ppm. ^{13}C NMR ($CDCl_3$, 125 MHz) δ: 161.9 (C-7), 151.6 (C-1), 150.2 (C-8), 145.9 (C-5), 135.2 (C-9), 129.5 (C-3), 128.6 (C12), 128.1 (C-10), 125.9 (C-11), 123.6 (C-6), 123.4 (C-4), 117.5 (C-13), 112.1 (C-2), 64.3 (CH_2), 40.3 $N(CH_3)_2$). HR-ESI-MS: *m*/*z* for $C_{18}H_{20}N_2O$ [M^+ +H]: 281.1648; found: 281.1646 (error 0.8532 ppm).

3-[3-(4-Dimethylaminophenyl)allylideneamino]benzyl alcohol (**1c**). The title compound was prepared from 4-dimethylamino-*trans*-cinnamaldehyde (1.75 g, 10 mmol) and 3-aminobenzyl

Electronic Supplementary Material (ESI) for New Journal of Chemistry
This journal is © The Royal Society of Chemistry and The Centre National de la Recherche Scientifique 2013

alcohol (1.23 g, 10 mmol) under reflux of methanol for 1.5 h, to give 2.42 g (8.6 mmol, 86% yield) of **1c**. m.p.: 149-150ºC. In solution the imine hydrolyses to the starting materials and therefore the spectra show the signals corresponding to the aldehyde and the aminobenzyl alcohol. IR (KBr) $\bar{\nu}_{max}$(cm^{-1}): 3184, 2918, 2857, 1605 (CN), 1563, 1482, 1365, 1230, 1151, 998, 930. ^{1}H NMR ($CDCl_3$, 500 MHz) δ: 8.22 (1H, d, *J* = 9.1 Hz, H-7), 7.44 (2H, d, *J* = 8.9 Hz, H-3), 7.34 (1H, t, *J* = 8.0 Hz, H-12), 7.25 (1H, s, H-9), 7.19 (1H, d, *J* = 7.0 Hz, H-13), 7.12 (1H, d, *J* = 5.5 Hz, H-11), 7.11 (1H, d, *J* = 5.5 Hz, H-5), 6.97 (1H, dd, *J* = 15.6, 9.1 Hz, H-6), 6.69 (2H, d, *J* = 8.9 Hz, H-2), 4.72 (2H, s, CH_2), 3.03 (6H, s, $N(CH_3)_2$) ppm. ^{13}C NMR ($CDCl_3$, 125 MHz) δ: 162.6 (C-7), 151.6 (C-1), 146.0 (C-8), 142.2 (C-10), 129.44 (C-12), 129.43 (C-3), 124.5 (C-9), 123.6 (C-4), 123.3 (C-6), 120.4 (C-13), 119.3 (C-11), 112.1 (C-2), 65.3 (CH_2), 40.3 ($N(CH_3)_2$). HR-ESI-MS: *m*/*z* for $C_{18}H_{21}N_2O$ [M^+ +H]: 281.1648; found: 281.1649 (error 0.2136 ppm).

4-[4-(4-Dimethylaminophenyl)allylideneamino]aminophenethyl alcohol (**1d**). The title compound was prepared from 4-dimethylamino-*trans*-cinnamaldehyde (1.00 g, 5.7 mmol) and 4-aminophenethyl alcohol (0.78 g, 6.3 mmol) under reflux of methanol for 1.5 h, to give 1.65 g (5.6 mmol, 98% yield) of **1d**. m.p.: 127-130ºC. IR (KBr) $\bar{\nu}_{max}$(cm^{-1}): 3098, 2904, 2861, 1599 (CN), 1564, 1362, 1227, 1154, 1048, 945, 810. ^{1}H NMR ($CDCl_3$, 500 MHz) δ: 8.21 (1H, d, *J* = 9.0 Hz, H-7), 7.43 (2H, d, *J* = 8.9 Hz, H-3), 7.22 (2H, d, *J* = 8.3 Hz, H-10), 7.13 (2H, d, *J* = 8.3 Hz, H-9), 7.07 (1H, d, *J* = 15.7 Hz, H-5), 6.94 (1H, dd, *J* = 15.7, 9.0 Hz, H-6), 6.69 (2H, d, *J* = 8.9 Hz, H-2), 3.86 (2H, t, *J* = 6.6 Hz, CH_2OH), 3.02 (6H, s, $N(CH_3)_2$), 2.87 (2H, t, *J* = 6.6 Hz, CH_2) ppm. ^{13}C NMR ($CDCl_3$, 125 MHz) δ: 162.2 (C-7), 151.5 (C-1), 150.3 (C-8), 145.3 (C-5), 136.1 (C-11), 129.9 (C-10), 129.3 (C-3), 123.7 (C-6), 123.6 (C-4), 121.2 (C-9), 112.1 (C-2), 63.7 (CH_2OH), 40.3 ($N(CH_3)_2$), 38.8 (CH_2). HR-ESI$^+$-MS: *m*/*z* for $C_{19}H_{22}N_2O$ [M^+ +H]: 295.1805; found: 2.1806 (error 0.3726 ppm).

(R)-(-)-2-[3-(4-Dimethylaminophenyl)allylideneamino]-phenyglycinol (**2a**). The title compound was prepared from 4-dimethylamino-*trans*-cinnamaldehyde (1.75 g, 10 mmol) and (R)-(-)-2-phenylglycinol (1.37 g, 10 mmol) under reflux of methanol for 1.5 h, to give 2.76 (9.38 mmol, 94% yield) of **2a**. m.p.: 174-175ºC. IR (KBr) $\bar{\nu}_{max}$(cm^{-1}): 3084, 3027, 2816, 1595 (CN), 1483, 1364, 1160, 964, 804. ^{1}H NMR ($CDCl_3$, 500 MHz) δ: 8.04 (1H, dd, *J* = 6.1, 2.6 Hz, H-7), 7.34 (2H, d, *J* = 9.0 Hz, H-11), 7.35-7.33 (4H, m, H-12, H-3), 7.25 (1H, t, *J* = 7.3 Hz, H-13), 6.82 (1H, s, H-6), 6.81 (1H, d, *J* = 6.1 Hz, H-5), 6.66 (2H, d, *J* = 9.0 Hz, H-2), 4.37 (1H, dd, *J* = 8.9, 4.2Hz, H-8), 3.99 (1H, dd, *J* = 11.5, 8.9 Hz, H-9A), 3.87 (1H, dd, *J* = 11.5, 4.2 Hz, H-9B), 3.00 (6H, s, $N(CH_3)_2$) ppm. ^{13}C NMR ($CDCl_3$, 125 MHz) δ: 165.7 (C-7), 151.4 (C-1), 144.6 (C-5), 140.8 (C-10), 129.2 (C-3), 128.7, 127.4 (C-12, C-11) 127.5 (C-13), 123.6 (C-4), 122.5 (C-6), 112.0 (C-2), 76.3 (C-8), 67.7 (C-

Electronic Supplementary Material (ESI) for New Journal of Chemistry
This journal is © The Royal Society of Chemistry and The Centre National de la Recherche Scientifique 2013

9), 40.3 ($N(CH_3)_2$). HR-ESI-MS: *m*/*z* for $C_{19}H_{22}N_2O$ [M^+ + H]: 295.1804; found: 295.1805 (error 0.0338 ppm).

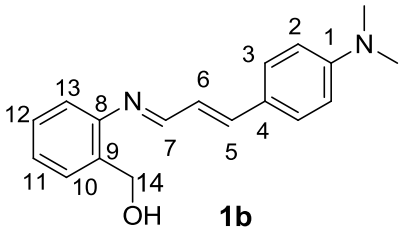
(1R,2S)-2-[(4-Dimethylaminophenyl)allylideneamino]-1-phenyl-1-propanol (**2b**). The title compound was prepared from 4-dimethylamino-*trans*-cinnamaldehyde (1.75 g, 10 mmol) and (1R,2S)-2-amino-1-phenyl-1-propanol (1.51 g, 10 mmol) under reflux of methanol for 1.5 h, to give 2.53 g (8.19 mmol, 82% yield) of **2b**. m.p.: 125-123ºC. IR (KBr) $\bar{\nu}_{max}$(cm^{-1}): 3152, 2981, 2853, 1590 (CN), 1521, 1359, 1266, 1158, 991, 808. ^{1}H NMR ($CDCl_3$, 500 MHz) δ: 7.95 (1H, d, *J* = 8.9 Hz, H-7), 7.40 (2H, d, *J* = 7.3 Hz, H-11), 7.34 (2H, t, *J* = 7.7 Hz, H-12), 7.27 (2H, d, *J* = 8.9 Hz, H-3), 7.26 (1H, t, *J* = 6.8 Hz, H-13), 6.83 (1H, d, *J* = 15.8 Hz, H-5), 6.69 (1H, dd, *J* = 15.8, 8.9 Hz, H-6), 6.64 (2H, d, *J* = 8.7 Hz, H-2), 4.81 (1H, d, *J* = 4.0 Hz, H-9), 3.47 (1H, m, H-8), 2.99 (6H, s, $N(CH_3)_2$), 1.11 (3H, d, *J* = 6.6 Hz H-14) ppm. ^{13}C NMR ($CDCl_3$, 125 MHz) δ: 163.2 (C-7), 151.1 (C-1), 143.3 (C-5),141.8 (C-10), 128.9 (C-3), 128.2 (C-12), 127.2 (C-11), 126.7 (C-13), 123.7 (C-4) 123.2 (C-6), 112.1 (C-2), 76.9 (C-9), 71.2 (C-8), 40.3($N(CH_3)_2$), 15.9 (C-14). HR-ESI-MS: *m*/*z* for $C_{20}H_{25}N_2O$ [M^+ +H]: 309.1961; found: 309.1968 (error 2.13 ppm).

2-((S)-3-(4-dimethylaminophenyl)allylideneamino)-1-butanol (**2c**). The title compound was prepared from 4-dimethylamino-*trans*-cinnamaldehyde (1.75 g, 10 mmol) and (S)-(-)-2-amino-1-butanol (0.89 g, 10 mmol) under reflux of methanol for 1.5 h, to give 2.04 g (8.28 mmol, 83% yield) of **2c**. M.P.: 140-138ºC. IR (KBr) $\bar{\nu}_{max}$(cm^{-1}): 3180, 2958, 2848, 1663, 1597 (CN), 1525, 1441, 1368, 1159, 1061, 980, 808. ^{1}H NMR ($CDCl_3$, 500 MHz) δ: 7.93 (1H, d, *J* = 8.8 Hz, H-7), 7.31 (1H, d, *J* = 8.6 Hz, H-3), 7.79 (1H, d, *J* = 15.9 Hz, H-5), 6.71 (1H, dd, *J* = 8.8, 15.9 Hz, H-6), 6.64 (2H, d, *J* = 8.8 Hz, H-2), 3.70 (2H, dd, *J* = 7.9, 7.5 Hz, H-9), 3.03 (1H, m, H-8), 2.99 (6H, s, $N(CH_3)_2$), 1.54 (2H, dq, *J* = 7.75 Hz, CH_2), 0.83 (3H, t, *J* = 7.5 Hz, CH_3) ppm. ^{13}C NMR ($CDCl_3$, 125 MHz) δ: 164.5 (C-7), 151.1 (C-1), 143.2 (C-5), 128.9 (C-3), 123.7 (C-4), 122.9 (C-6), 112.1 (C-2), 74.5 (C-8) 66.2 (C-9), 40.3 ($N(CH_3)_2$), 25.3 (CH_2), 10.9 (CH_3) ppm. HR-ESI-MS: *m*/*z* for $C_{15}H_{24}N_2O$ [M^+ +H]: 247.1805; found: 247.1807 (error 0.8495 ppm).

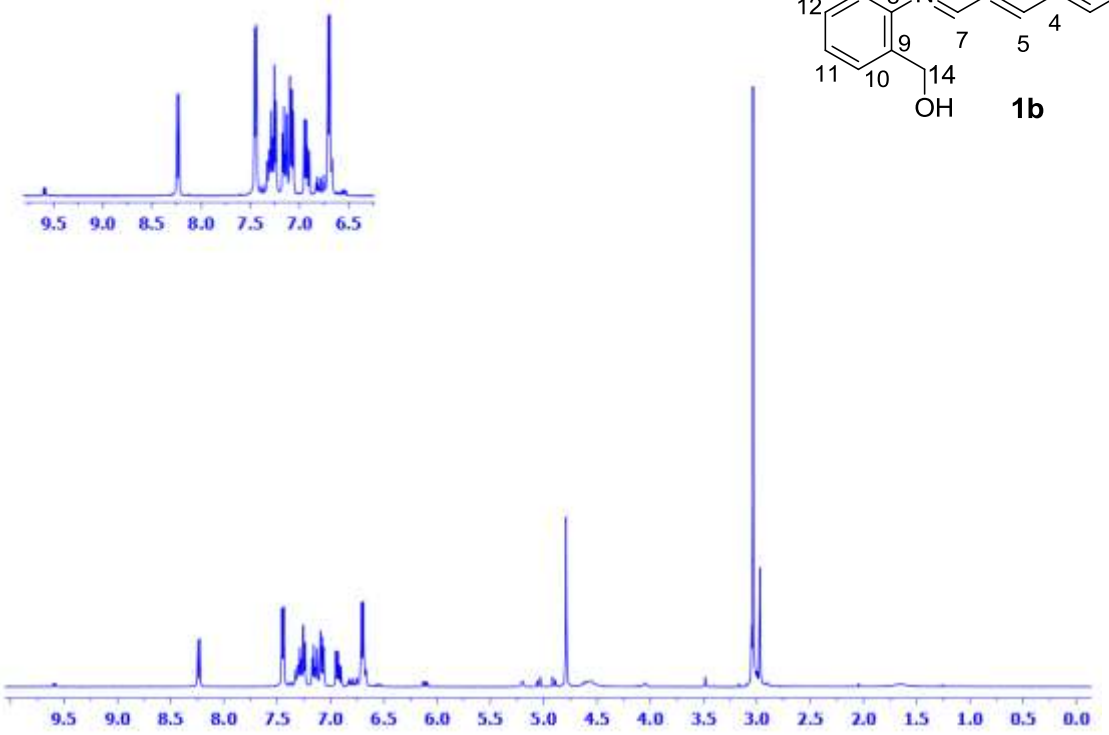
Electronic Supplementary Material (ESI) for New Journal of Chemistry
This journal is © The Royal Society of Chemistry and The Centre National de la Recherche Scientifique 2013

II ^{1}H and ^{13}C NMR spectra of compounds 1b – 1d, 2a – 2c

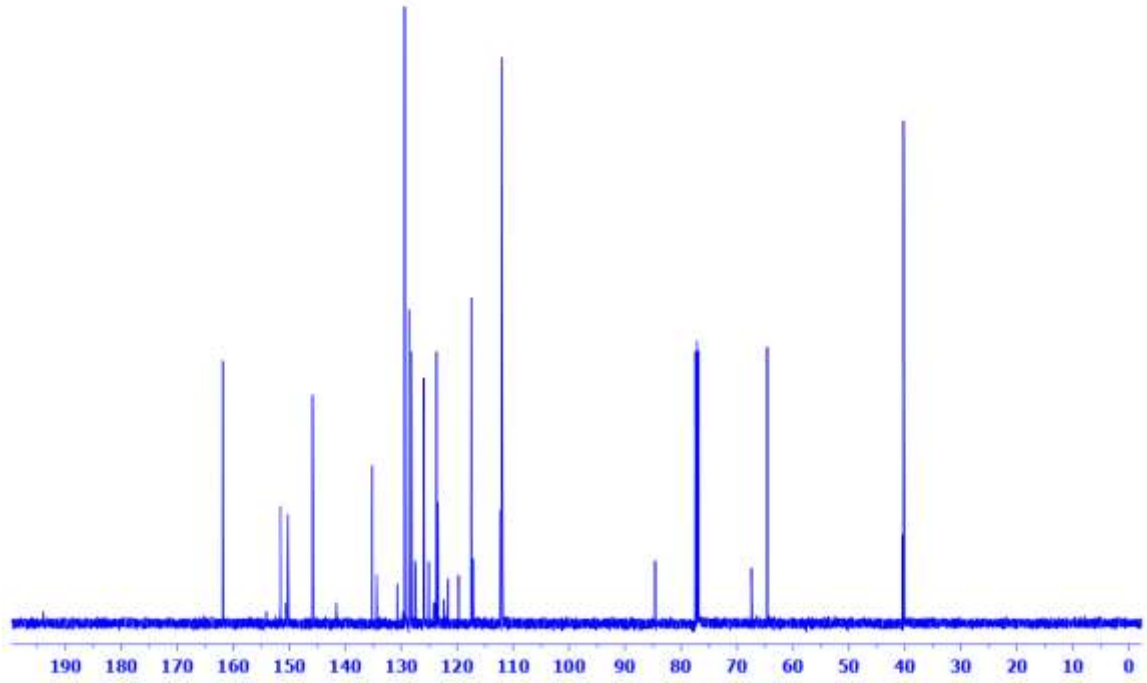
Schiff base 1b:



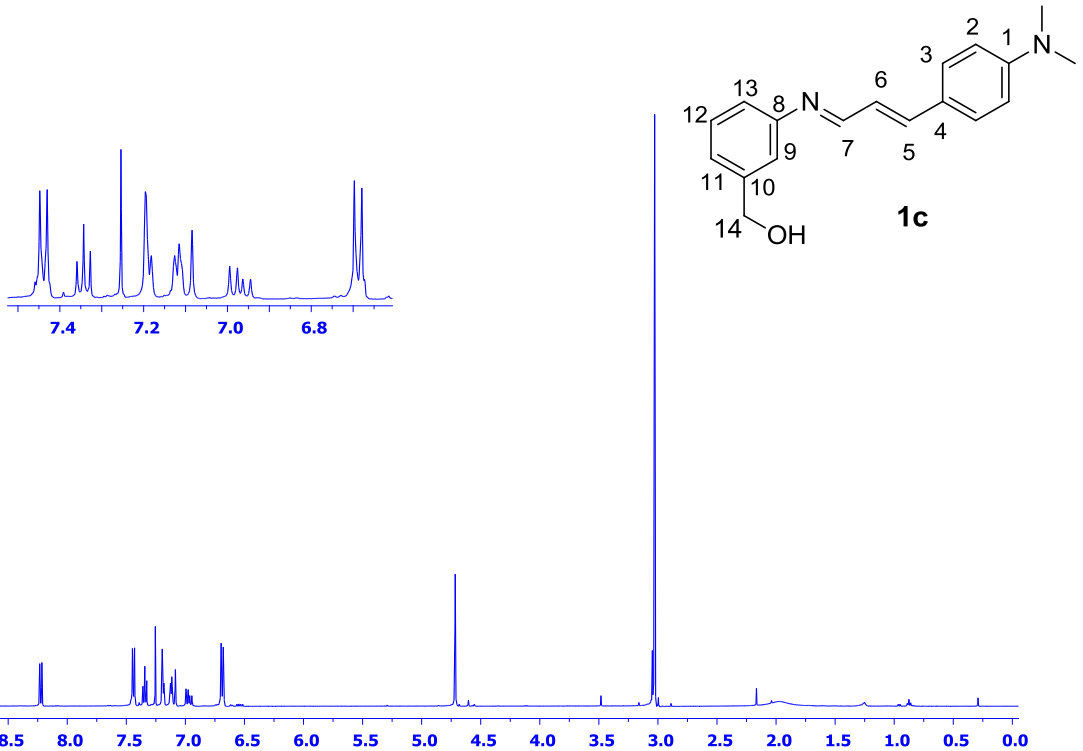
1b



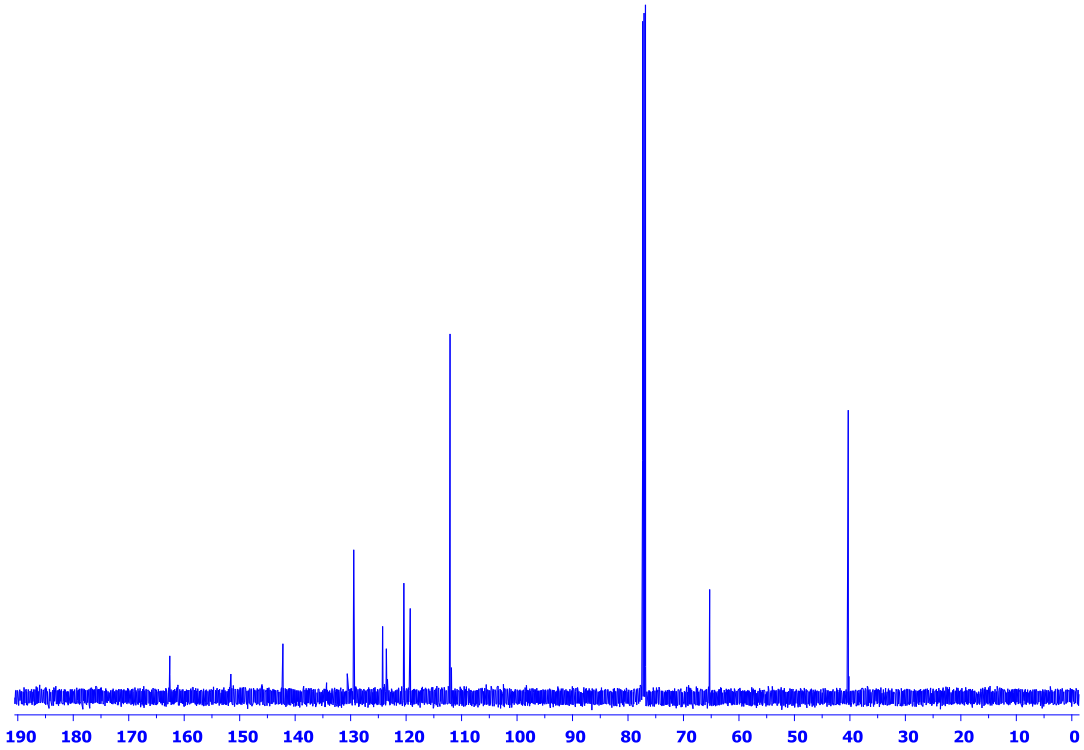
Supplementary Material (ESI) for New Journal of Chemistry
This journal is (c) The Royal Society of Chemistry and The Centre National de la Recherche Scientifique, 2012.



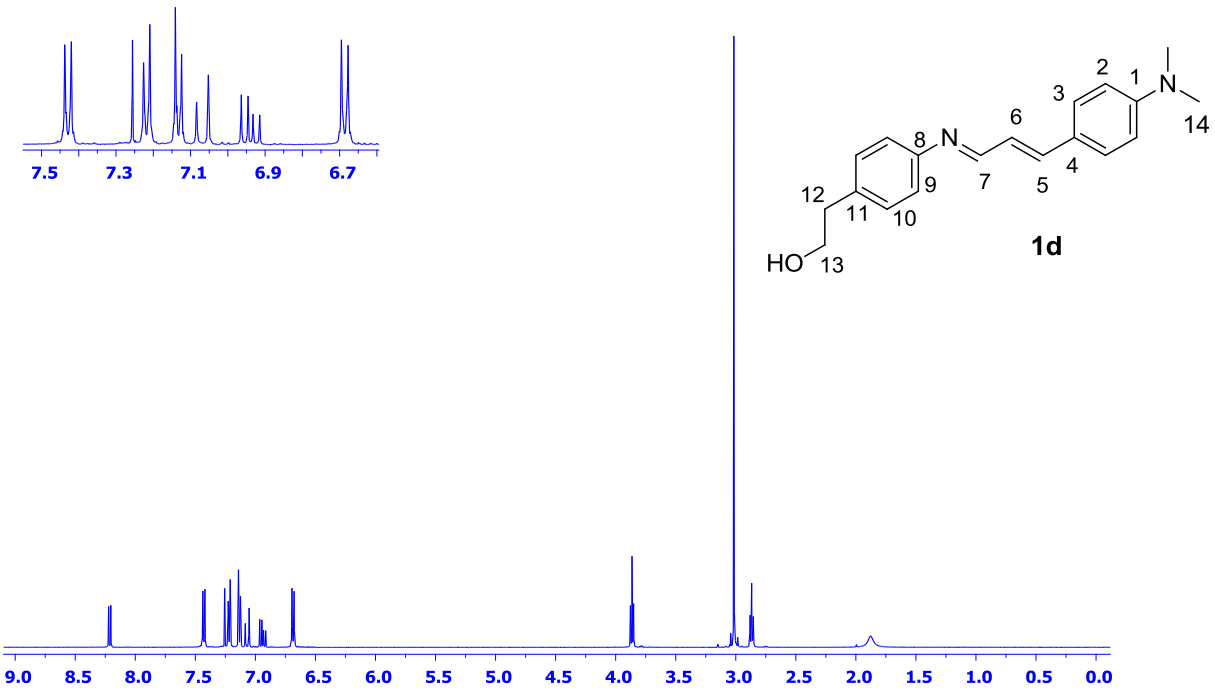
Schiff base 1c:



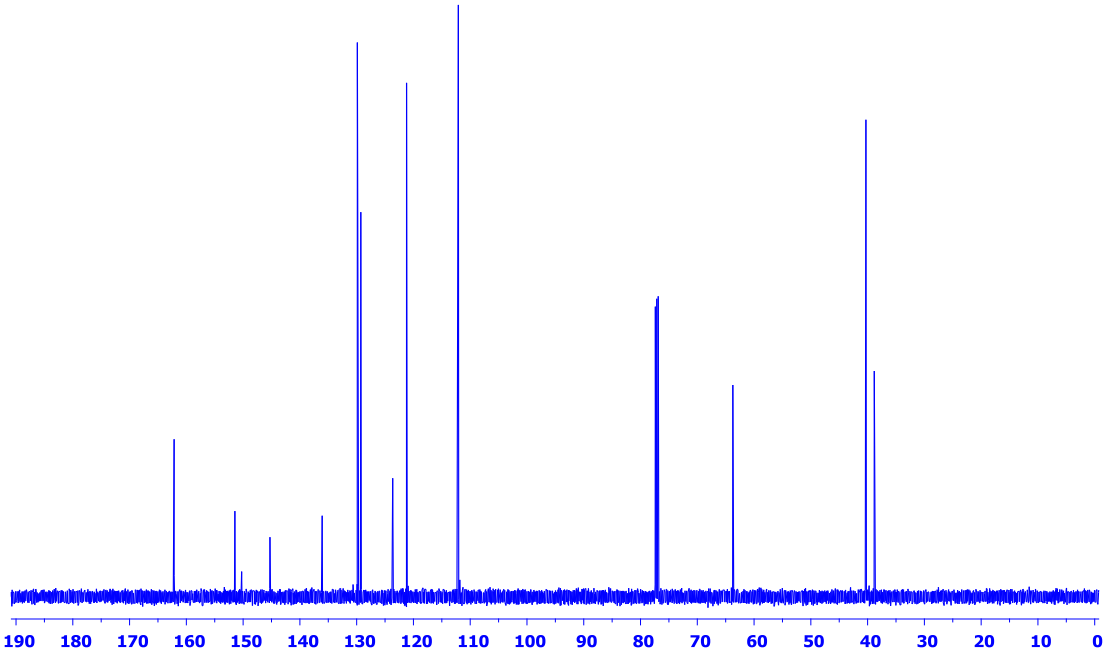
Supplementary Material (ESI) for New Journal of Chemistry
This journal is (c) The Royal Society of Chemistry and The Centre National de la Recherche Scientifique, 2012.



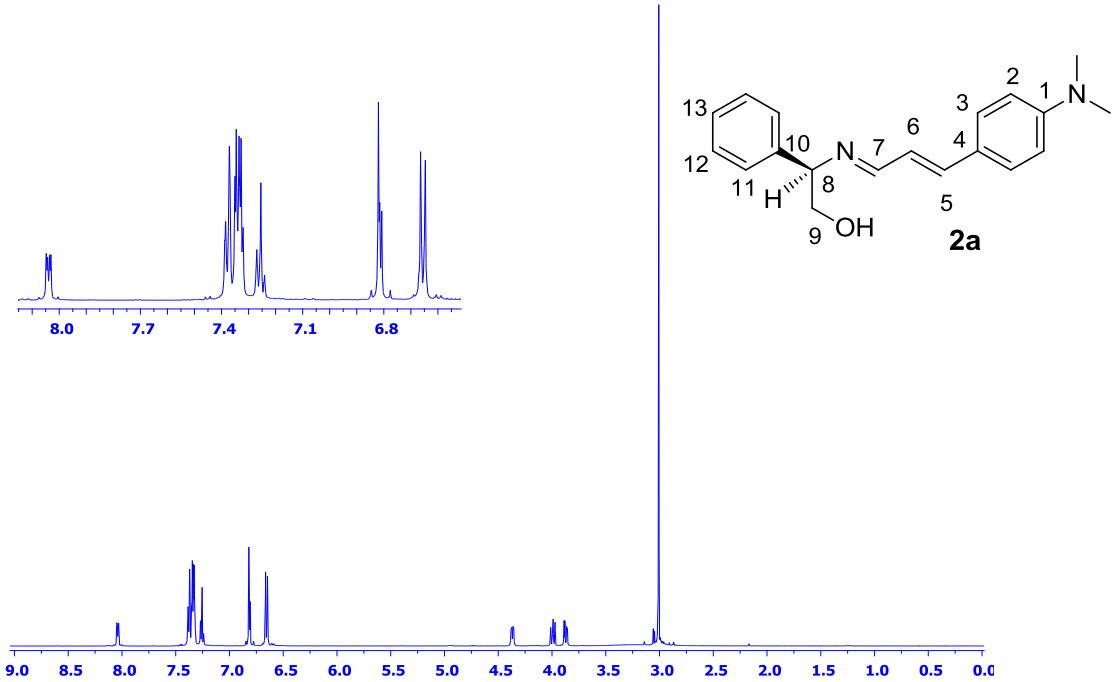
Schiff base 1d:



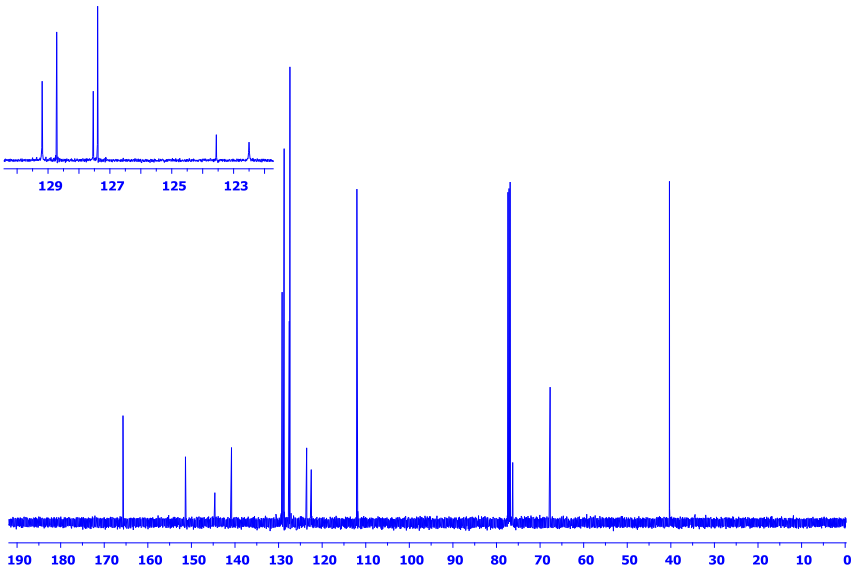
Supplementary Material (ESI) for New Journal of Chemistry
This journal is (c) The Royal Society of Chemistry and The Centre National de la Recherche Scientifique, 2012.



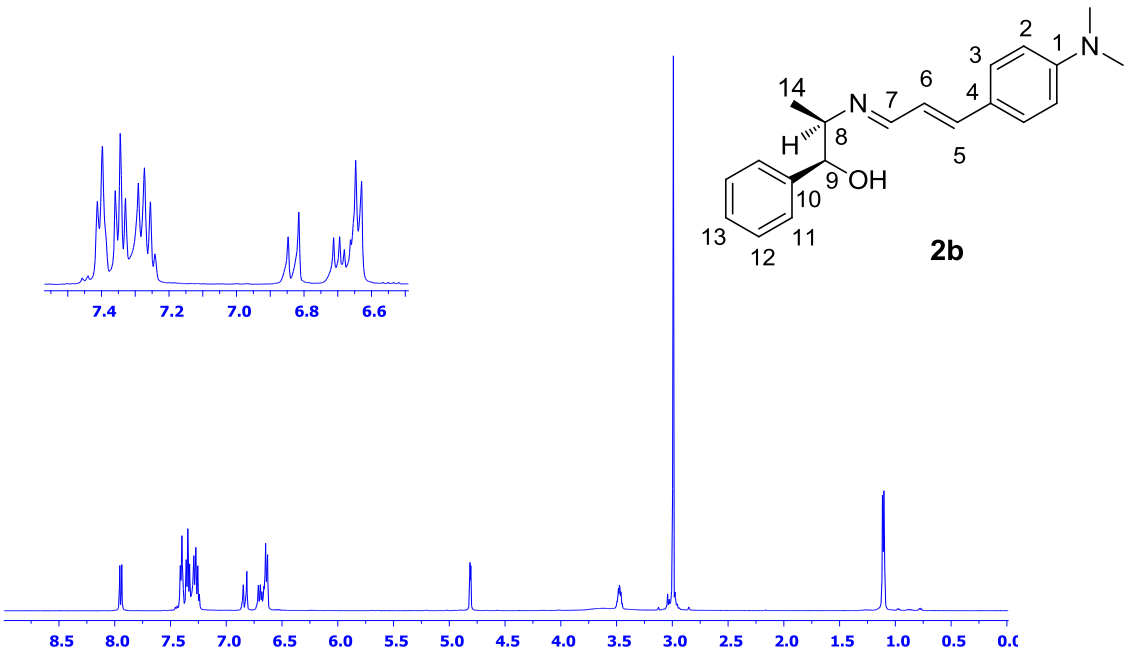
Schiff base 2a:



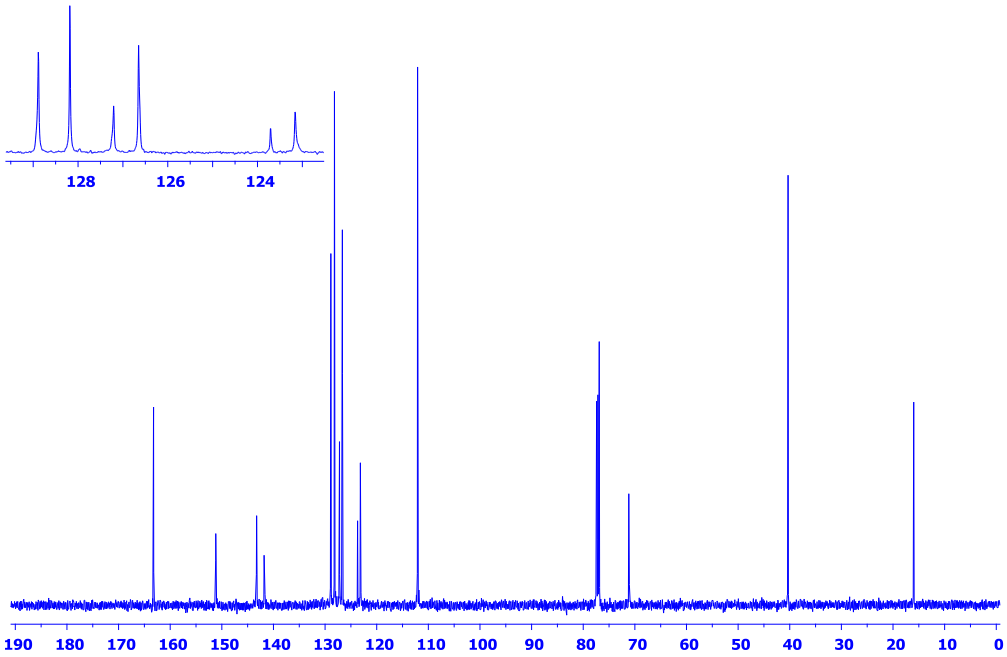
Supplementary Material (ESI) for New Journal of Chemistry
This journal is (c) The Royal Society of Chemistry and The Centre National de la Recherche Scientifique, 2012.



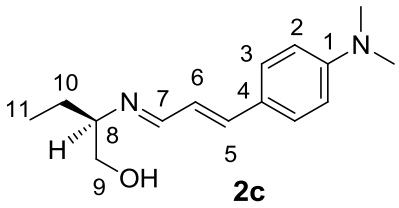
Schiff base 2b:



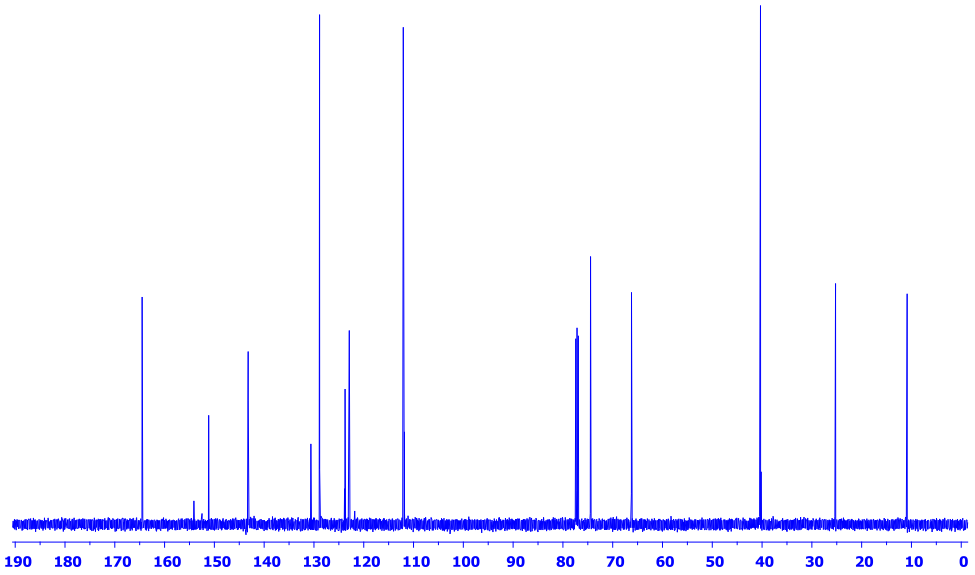
Supplementary Material (ESI) for New Journal of Chemistry
This journal is (c) The Royal Society of Chemistry and The Centre National de la Recherche Scientifique, 2012.



Schiff base 2c:



2c



III Crystal data and bond length and angles of compounds 1b, 1c and 2a

Table S1 Summary of crystal data at 293 K

Compound	1b	1c	2a
Crystal color	Yellow	Red	Yellow
Empirical formula	$C_{18}H_{20}N_2O$	$C_{18}H_{20}N_2O$	$C_{19}H_{22}N_2O$
Mol wt.	280.36	280.36	294.39
Crystal System	Orthorhombic	Orthorhombic	Monoclinic
Space group	$P2_12_12_1$	$Pca2_1$	$P2_1$
a (Å)	6.1828(2)	7.8065(4)	10.1300(0)
b (Å)	14.6917(8)	16.4260(14)	6.3550(0)
c (Å)	16.9541(5)	12.1222(12)	13.5220(0)
α (°)	90	90	90
β (°)	90	90	90
γ (°)	90	90	105.715(0)
V (Å^3)	1540.04(1)	1554.4(2)	837.96(0)
Z	4	4	2
$\rho_{calcd.}$ (g/cm^3)	1.209	1.198	1.110
Θ Range (°)	27.485	19.98	27.50
F(000)	599.9	599.9	299.9
Abs. Coeff. (mm$^-$	0.076	0.075	0.069
No. of reflections:			
Measured	11063	3602	5581
Unique	3393	1418	3286
Observed	2339	1248	2830
R [I > 2σ(I)]	0.054	0.038	0.046
Rw (all data)	0.0943	0.106	0.089
Parameters	196	190	203
ρ_{min} (e Å^3)	-0.156	-0.098	-0.147
ρmax (e Å3)	0.118	0.082	0.121
GOOF	1.039	0.976	1.026

Electronic Supplementary Material (ESI) for New Journal of Chemistry
This journal is © The Royal Society of Chemistry and The Centre National de la Recherche Scientifique 2013

Compound 1b:

Bond lengths [Å] and angles [°]

C(1)-N(2)	1.377(3)
C(1)-C(2)	1.395(3)
C(1)-C(2A)	1.399(3)
C(2)-C(3)	1.370(3)
C(2A)-C(3A)	1.374(3)
C(3)-C(4)	1.396(3)
C(3A)-C(4)	1.395(3)
C(4)-C(5)	1.448(3)
C(5)-C(6)	1.335(3)
C(6)-C(7)	1.435(3)
C(7)-N(1)	1.289(3)
C(8)-C(13)	1.385(3)
C(8)-C(9)	1.400(3)
C(8)-N(1)	1.417(3)
C(9)-C(10)	1.385(3)
C(9)-C(14)	1.503(3)
C(10)-C(11)	1.377(4)
C(11)-C(12)	1.368(4)
C(12)-C(13)	1.377(4)
C(14)-O(1)	1.423(3)
C(15)-N(2)	1.439(3)
C(15A)-N(2)	1.424(4)

N(2)-C(1)-C(2)	121.7(2)
N(2)-C(1)-C(2A)	121.6(2)
C(2)-C(1)-C(2A)	116.7(2)
C(3)-C(2)-C(1)	121.1(2)
C(3A)-C(2A)-C(1)	121.6(2)
C(2)-C(3)-C(4)	122.8(2)
C(2A)-C(3A)-C(4)	122.0(2)
C(3A)-C(4)-C(3)	115.8(2)
C(3A)-C(4)-C(5)	124.2(2)
C(3)-C(4)-C(5)	119.91(19)
C(6)-C(5)-C(4)	128.4(2)
C(5)-C(6)-C(7)	121.5(2)
N(1)-C(7)-C(6)	122.9(2)
C(13)-C(8)-C(9)	119.7(2)
C(13)-C(8)-N(1)	116.7(2)
C(9)-C(8)-N(1)	123.54(19)
C(10)-C(9)-C(8)	117.9(2)
C(10)-C(9)-C(14)	118.6(2)
C(8)-C(9)-C(14)	123.39(19)
C(11)-C(10)-C(9)	122.1(2)
C(12)-C(11)-C(10)	119.4(2)
C(11)-C(12)-C(13)	120.1(2)
C(12)-C(13)-C(8)	120.8(2)
O(1)-C(14)-C(9)	113.0(2)
C(7)-N(1)-C(8)	120.54(18)

Electronic Supplementary Material (ESI) for New Journal of Chemistry
This journal is © The Royal Society of Chemistry and The Centre National de la Recherche Scientifique 2013

C(1)-N(2)-C(15A)	121.4(2)
C(1)-N(2)-C(15)	120.8(2)
C(15A)-N(2)-C(15)	117.6(2)

Torsion angles [°]

C(13)-C(8)-N(1)-C(7)	-131.5(2)
C(9)-C(8)-N(1)-C(7)	52.9(3)
N(1)-C(7)-C(6)-C(5)	-178.0(2)
C(2A)-C(1)-N(2)-C(15A)	0.8(4)
C(2)-C(1)-N(2)-C(15)	-3.7(4)
C(9)-C(14)-O(1)-H(1)	-109(2)

Hydrogen bonds [Å and °].

D-H...A	d(D-H)	d(H...A)	d(D...A)	<(DHA)
O(1)-H(1)...N(1)#1	0.96(4)	1.84(4)	2.774(2)	163(3)

Symmetry transformations used to generate equivalent atoms:
#1 x-1,y,z

Compound 1c:

Bond lengths [Å] and angles [°].

C(1)-N(2)	1.375(5)
C(1)-C(2A)	1.391(5)
C(1)-C(2)	1.397(5)
C(2)-C(3)	1.367(5)
C(2A)-C(3A)	1.367(5)
C(3)-C(4)	1.394(5)
C(3A)-C(4)	1.382(5)
C(4)-C(5)	1.454(5)
C(5)-C(6)	1.339(5)
C(6)-C(7)	1.422(5)
C(7)-N(1)	1.288(4)
C(8)-C(13)	1.387(5)
C(8)-C(9)	1.396(5)
C(8)-N(1)	1.416(5)
C(9)-C(10)	1.381(5)
C(10)-C(11)	1.391(5)
C(10)-C(14)	1.490(5)
C(11)-C(12)	1.371(5)
C(12)-C(13)	1.383(5)
C(14)-O(1)	1.415(4)
C(15)-N(2)	1.434(6)
C(15A)-N(2)	1.444(5)

N(2)-C(1)-C(2A)	120.8(4)
N(2)-C(1)-C(2)	121.9(4)
C(2A)-C(1)-C(2)	117.3(3)
C(3)-C(2)-C(1)	120.9(3)
C(3A)-C(2A)-C(1)	120.8(3)

Electronic Supplementary Material (ESI) for New Journal of Chemistry
This journal is © The Royal Society of Chemistry and The Centre National de la Recherche Scientifique 2013

C(2)-C(3)-C(4)	122.0(3)
C(2A)-C(3A)-C(4)	122.6(3)
C(3A)-C(4)-C(3)	116.3(3)
C(3A)-C(4)-C(5)	122.3(3)
C(3)-C(4)-C(5)	121.4(3)
C(6)-C(5)-C(4)	127.9(3)
C(5)-C(6)-C(7)	123.0(3)
N(1)-C(7)-C(6)	122.2(3)
C(13)-C(8)-C(9)	118.9(3)
C(13)-C(8)-N(1)	118.5(3)
C(9)-C(8)-N(1)	122.4(3)
C(10)-C(9)-C(8)	121.4(3)
C(9)-C(10)-C(11)	118.2(3)
C(9)-C(10)-C(14)	120.4(3)
C(11)-C(10)-C(14)	121.4(3)
C(12)-C(11)-C(10)	121.1(3)
C(11)-C(12)-C(13)	120.2(4)
C(12)-C(13)-C(8)	120.0(4)
O(1)-C(14)-C(10)	113.7(3)
C(7)-N(1)-C(8)	120.5(3)
C(1)-N(2)-C(15)	122.5(4)
C(1)-N(2)-C(15A)	120.2(4)
C(15)-N(2)-C(15A)	117.3(4)

Torsion angles [°].

C(8)-C(13)-C(7)-N(1)	98.6(6)
N(1)-C(7)-C(6)-C(5)	179.4(3)
C(2)-C(1)-N(2)-C(15)	-0.4(6)
C(2A)-C(1)-N(2)-C(15A)	-4.3(5)
C(10)-C(14)-O(1)-H(1)	55.5

Hydrogen bonds [Å and °].

D-H...A	d(D-H)	d(H...A)	d(D...A)	<(DHA)
O(1)-H(1A)...N(1)#1	0.82	2.04	2.849(4)	167.1

Symmetry transformations used to generate equivalent atoms:
#1 x+1/2,-y+1,-z

Compound 2a:

Bond lengths [Å] and angles [°].

C(1)-N(2)	1.3785(19)
C(1)-C(2)	1.397(2)
C(1)-C(2A)	1.408(2)
C(2)-C(3)	1.382(2)
C(2)-H(2)	0.9300
C(2A)-C(3A)	1.380(2)
C(2A)-H(2A)	0.9300
C(3)-C(4)	1.399(2)
C(3)-H(3)	0.9300

Electronic Supplementary Material (ESI) for New Journal of Chemistry
This journal is © The Royal Society of Chemistry and The Centre National de la Recherche Scientifique 2013

C(3A)-C(4)	1.399(2)
C(3A)-H(3A)	0.9300
C(4)-C(5)	1.4510(19)
C(5)-C(6)	1.345(2)
C(5)-H(5)	0.9300
C(6)-C(7)	1.4396(19)
C(6)-H(6)	0.9300
C(7)-N(1)	1.2774(18)
C(7)-H(7)	0.9300
C(8)-N(1)	1.4719(18)
C(8)-C(10)	1.5186(19)
C(8)-C(9)	1.5282(19)
C(8)-H(8)	0.9800
C(9)-O(1)	1.4133(17)
C(9)-H(9A)	0.9700
C(9)-H(9B)	0.9700
C(10)-C(11)	1.385(2)
C(10)-C(11A)	1.386(2)
C(11)-C(12)	1.397(2)
C(11)-H(11)	0.9300
C(11A)-C(12A)	1.387(2)
C(11A)-H(11A)	0.9300
C(12)-C(13)	1.369(4)
C(12)-H(12)	0.9300
C(12A)-C(13)	1.370(3)
C(12A)-H(12A)	0.9300
C(13)-H(13)	0.9300
C(14)-N(2)	1.453(2)
C(14)-H(14A)	0.9600
C(14)-H(14B)	0.9600
C(14)-H(14C)	0.9600
C(14A)-N(2)	1.431(3)
C(14A)-H(14D)	0.9600
C(14A)-H(14E)	0.9600
C(14A)-H(14F)	0.9600
O(1)-H(15)	0.85(2)

N(2)-C(1)-C(2)	121.14(14)
N(2)-C(1)-C(2A)	121.49(15)
C(2)-C(1)-C(2A)	117.36(13)
C(3)-C(2)-C(1)	120.92(14)
C(3)-C(2)-H(2)	119.5
C(1)-C(2)-H(2)	119.5
C(3A)-C(2A)-C(1)	120.85(14)
C(3A)-C(2A)-H(2A)	119.6
C(1)-C(2A)-H(2A)	119.6
C(2)-C(3)-C(4)	122.38(15)
C(2)-C(3)-H(3)	118.8
C(4)-C(3)-H(3)	118.8
C(2A)-C(3A)-C(4)	122.28(13)
C(2A)-C(3A)-H(3A)	118.9
C(4)-C(3A)-H(3A)	118.9
C(3)-C(4)-C(3A)	116.20(12)
C(3)-C(4)-C(5)	119.41(14)

Electronic Supplementary Material (ESI) for New Journal of Chemistry
This journal is © The Royal Society of Chemistry and The Centre National de la Recherche Scientifique 2013

C(3A)-C(4)-C(5)	124.39(13)
C(6)-C(5)-C(4)	128.17(15)
C(6)-C(5)-H(5)	115.9
C(4)-C(5)-H(5)	115.9
C(5)-C(6)-C(7)	121.69(15)
C(5)-C(6)-H(6)	119.2
C(7)-C(6)-H(6)	119.2
N(1)-C(7)-C(6)	122.81(14)
N(1)-C(7)-H(7)	118.6
C(6)-C(7)-H(7)	118.6
N(1)-C(8)-C(10)	110.63(11)
N(1)-C(8)-C(9)	109.27(12)
C(10)-C(8)-C(9)	109.13(11)
N(1)-C(8)-H(8)	109.3
C(10)-C(8)-H(8)	109.3
C(9)-C(8)-H(8)	109.3
O(1)-C(9)-C(8)	113.53(12)
O(1)-C(9)-H(9A)	108.9
C(8)-C(9)-H(9A)	108.9
O(1)-C(9)-H(9B)	108.9
C(8)-C(9)-H(9B)	108.9
H(9A)-C(9)-H(9B)	107.7
C(11)-C(10)-C(11A)	118.96(14)
C(11)-C(10)-C(8)	119.04(15)
C(11A)-C(10)-C(8)	121.98(14)
C(10)-C(11)-C(12)	119.84(19)
C(10)-C(11)-H(11)	120.1
C(12)-C(11)-H(11)	120.1
C(10)-C(11A)-C(12A)	120.60(18)
C(10)-C(11A)-H(11A)	119.7
C(12A)-C(11A)-H(11A)	119.7
C(13)-C(12)-C(11)	120.41(19)
C(13)-C(12)-H(12)	119.8
C(11)-C(12)-H(12)	119.8
C(13)-C(12A)-C(11A)	120.1(2)
C(13)-C(12A)-H(12A)	120.0
C(11A)-C(12A)-H(12A)	120.0
C(12)-C(13)-C(12A)	120.08(17)
C(12)-C(13)-H(13)	120.0
C(12A)-C(13)-H(13)	120.0
N(2)-C(14)-H(14A)	109.5
N(2)-C(14)-H(14B)	109.5
H(14A)-C(14)-H(14B)	109.5
N(2)-C(14)-H(14C)	109.5
H(14A)-C(14)-H(14C)	109.5
H(14B)-C(14)-H(14C)	109.5
N(2)-C(14A)-H(14D)	109.5
N(2)-C(14A)-H(14E)	109.5
H(14D)-C(14A)-H(14E)	109.5
N(2)-C(14A)-H(14F)	109.5
H(14D)-C(14A)-H(14F)	109.5
H(14E)-C(14A)-H(14F)	109.5
C(7)-N(1)-C(8)	117.23(13)
C(1)-N(2)-C(14A)	121.51(15)

Electronic Supplementary Material (ESI) for New Journal of Chemistry
This journal is © The Royal Society of Chemistry and The Centre National de la Recherche Scientifique 2013

C(1)-N(2)-C(14)	119.39(16)
C(14A)-N(2)-C(14)	118.71(14)
C(9)-O(1)-H(15)	108.7(13)

Torsion angles [°].

C(11A)-C(10)-C(8)-N(1)	34.87(17)
C(11)-C(10)-C(8)-C(9)	93.27(15)
N(1)-C(8)-C(9)-O(1)	60.84(15)
N(1)-C(7)-C(6)-C(5)	-178.12(13)
C(6)-C(5)-C(4)-C(3)	174.49(13)
C(2A)-C(1)-N(2)-C(14A)	5.7(2)

Hydrogen bonds [Å and °].

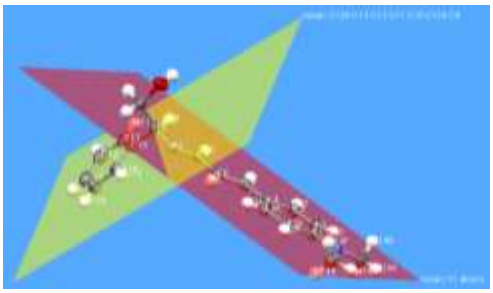
D-H...A	d(D-H)	d(H...A)	d(D...A)	<(DHA)
O(1)-H(15)...N(1)#1	0.85(2)	1.92(2)	2.7598(19)	169.7(18)

Symmetry transformations used to generate equivalent atoms:
#1 -x+2,y+1/2,-z+2

Electronic Supplementary Material (ESI) for New Journal of Chemistry
This journal is © The Royal Society of Chemistry and The Centre National de la Recherche Scientifique 2013

IV Spacefill representation of crystal packing and supramolecular arrangements

(a)



(b)

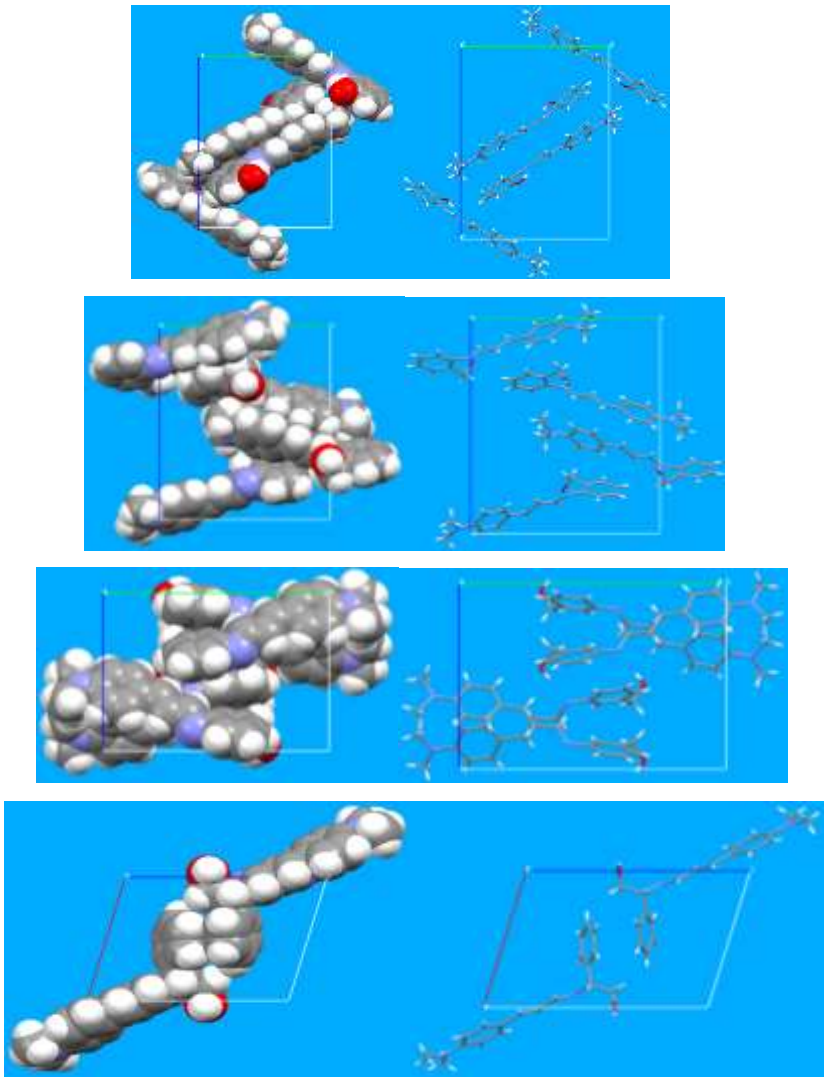


Fig. S1. (a) Illustration of A and B planes. (b) Spacefill and capped sticks representation of crystal packing of -from top to bottom- **1a**, **1b** and **1c** along the *a* axis and **2a** along the *b* axis, showing the open structure packing for **2a**.

Electronic Supplementary Material (ESI) for New Journal of Chemistry
This journal is © The Royal Society of Chemistry and The Centre National de la Recherche Scientifique 2013

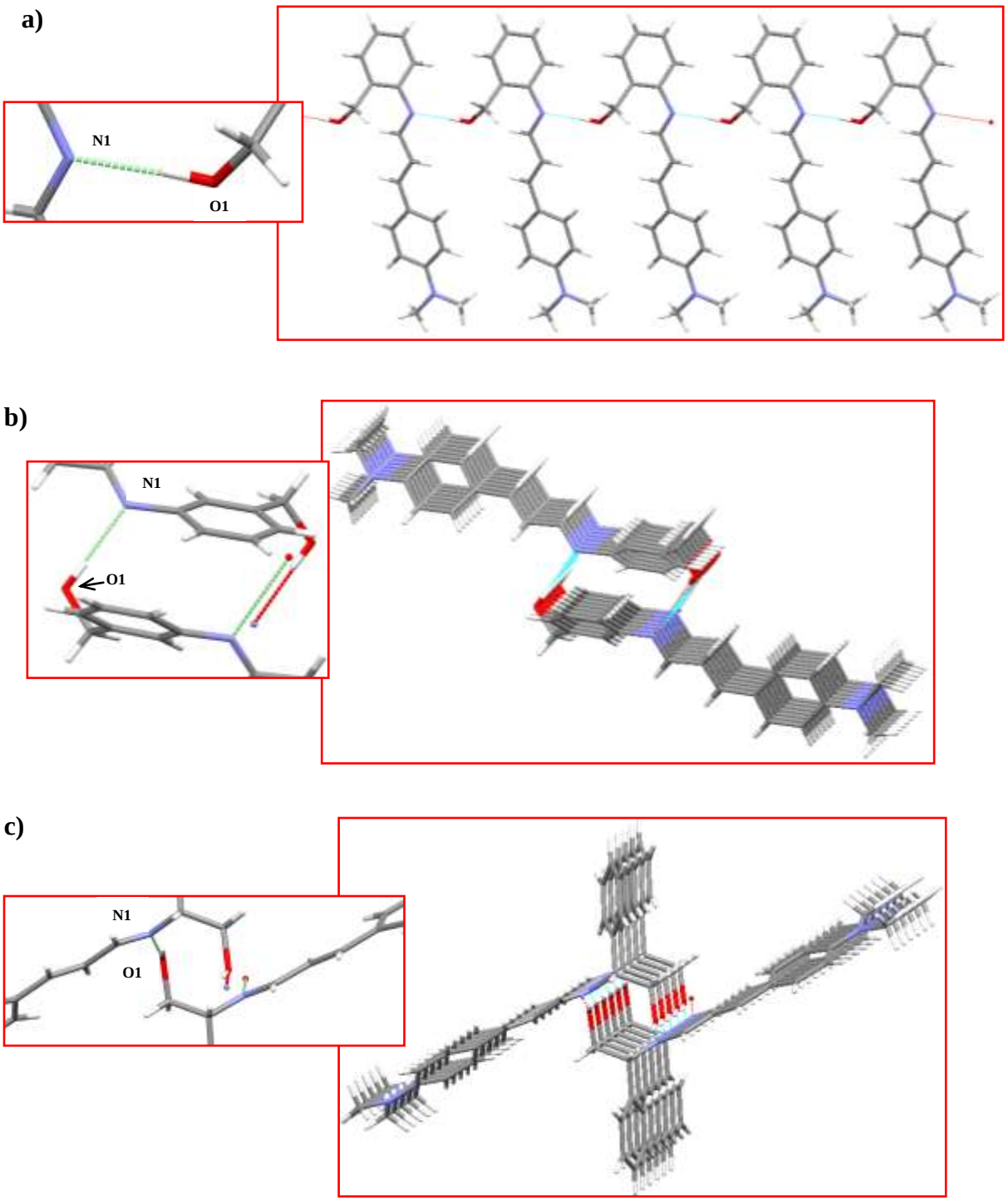


Fig. S2 Found hydrogen bond interactions in the crystal structure. a) **1b**, *O-H···N(C)=C* interaction along the *c* axis. b) **1c**, *O-H···N(C)=C* interaction along the *a* axis.d) **2a**, *O-H···N(C)=C* interaction along the *b* axis.

Electronic Supplementary Material (ESI) for New Journal of Chemistry
This journal is © The Royal Society of Chemistry and The Centre National de la Recherche Scientifique 2013

V Table S2. Catalán solvent parameters {SA, SB, SP, SdP}

	SP	SdP	SA	SB	Abs	Em	SS
Cyclohexane	0.683	0	0	0.073	28409.0909	24875.6219	3533.46902
Dioxane	0.737	0.312	0	0.444	28248.5876	24038.4615	4210.12603
Toluene	0.782	0.284	0	0.128	27855.1532	24038.4615	3816.69166
Diethyl ether	0.617	0.385	0	0.562	28571.1331	24213.0135	4358.16472
Ethyl acetate	0.656	0.603	0	0.542	28089.9721	23264.2013	4725.9848
THF	0.714	0.634	0	0.591	28248.5876	23419.2038	4829.38382
Octanol	0.713	0.454	0.299	0.923	27548.2094	23310.0233	4238.18606
Butanol	0.674	0.655	0.341	0.809	27700.1156	22521.9802	5178.1546
2-Propanol	0.633	0.808	0.283	0.83	27700.831	22727.2727	4973.55829
1-Propanol	0.658	0.748	0.367	0.782	27700.831	22522.5225	5178.3085
Acetone	0.651	0.907	0	0.475	28248.5876	22371.3647	5877.22292
EtOH	0.633	0.783	0.4	0.658	27472.5275	22172.949	5299.57847
MeOH	0.608	0.904	0.605	0.545	27397.2603	22075.0552	5322.20508
ACN	0.645	0.974	0.044	0.286	28089.8876	22026.4317	6063.45592
DMF	0.759	0.977	0.031	0.613	27932.9796	22172.0487	5760.9965
DMSO	0.830	1	0.072	0.647	28011.0186	21965.1103	6046.0782

Electronic Supplementary Material (ESI) for New Journal of Chemistry
This journal is © The Royal Society of Chemistry and The Centre National de la Recherche Scientifique 2013

VI Lippert plots for compound 2a

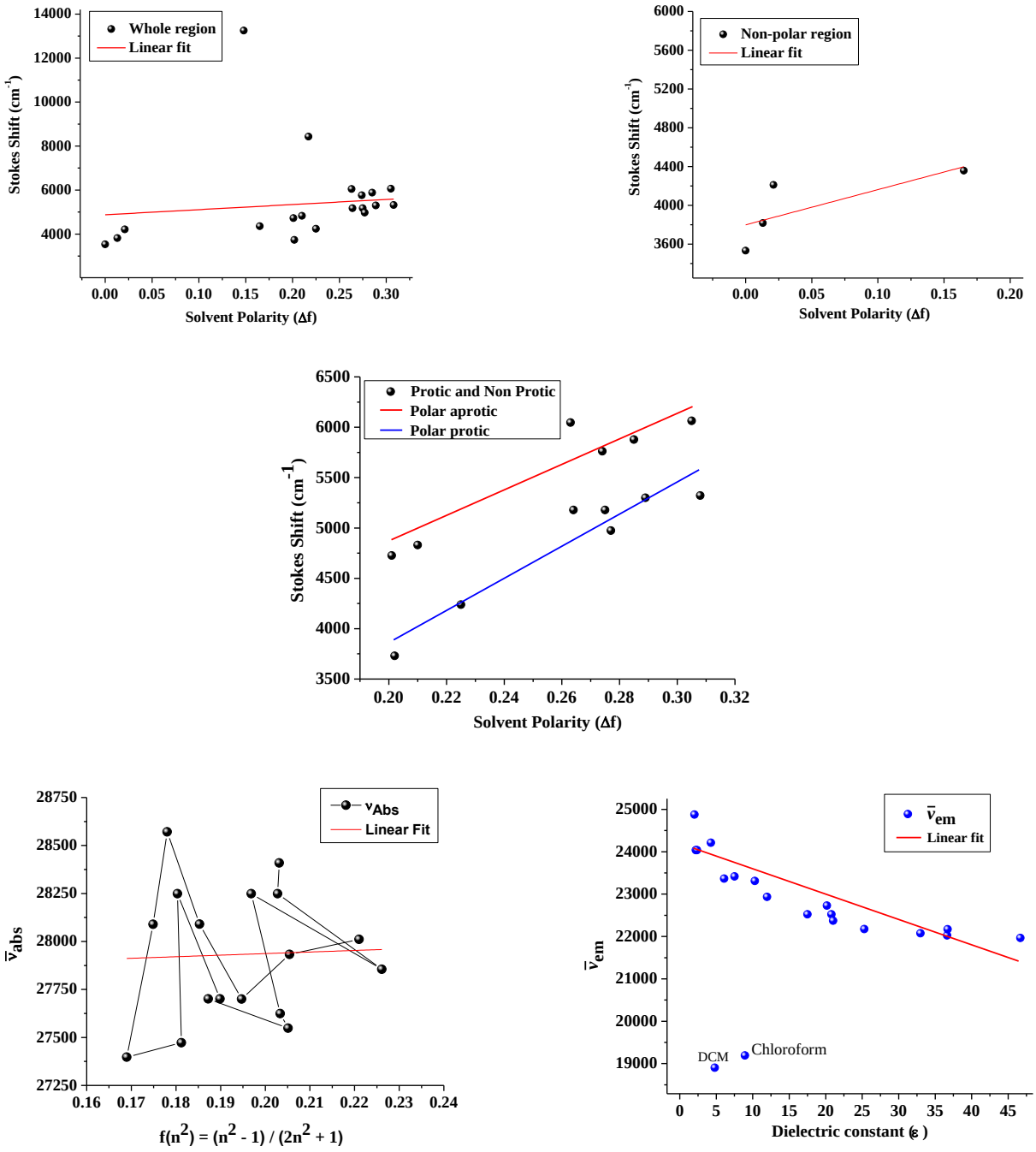


Fig. S3 Lippert-Mataga Plots for compound **2a**:

VII UV-vis spectra obtained by aggregation of 0.6 ml of a Acetic acid : ACN solution (1 : 99, v/v)

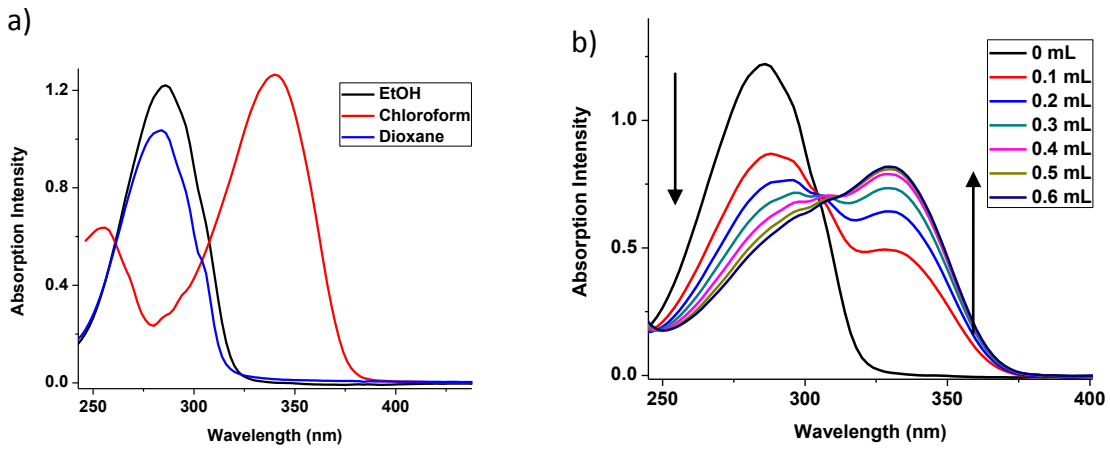


Fig. S4. UV-vis absorption spectra of molecule **3** in a) Ethanol, chloroform and dioxane solvents, b) acetic acid : ACN (1 : 99, v/v) solution.

Supplementary Material (ESI) for New Journal of Chemistry
This journal is (c) The Royal Society of Chemistry and The Centre National de la Recherche Scientifique, 2012.

VIII Experimental and calculated infrared spectra of 2a

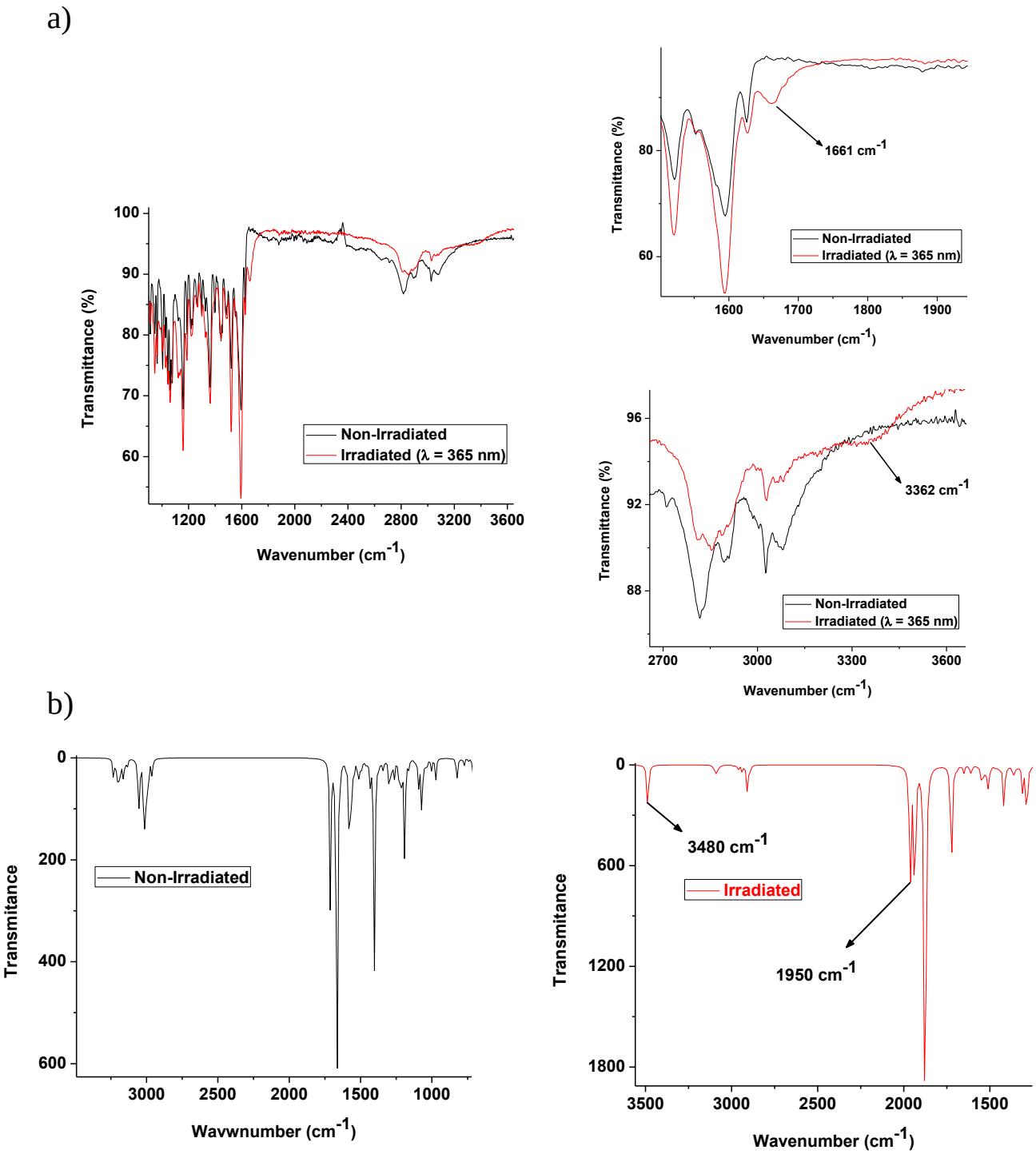


Fig. S4. Infrared spectra of **2a**: a) non-irradiated and irradiated by 365 nm light under 5 min; b) calculated vibrational frequencies at DFT (B3LYP/6-31G(d)). *Note*: The wavenumber axis has not been scaled by any factor.